# ARTICLE 07 NIN COUPLING VALUES IN n=2 AND OXYGEN ELECTRONIC DENSITY **Javier Silvestre** (eeatom.blogspot com)

# **ABSTRACT**

P34 NIN III: ns electron as origin of lobes in same n by curves coupling [6] is used to obtain z,  $C_{POTI-AL}$  and  $C_{PEP}$  in n=2. These values are used in later studies and are applied here to estimate maximum Oxygen electron density with simple method. Estimate must corroborate Fluorine example that is in agreement with references [6].

By this method, Probability  $(P_i)$  calculations are directed to delimited  $r_i$  (Electronic extremes-nucleus radial distance) differentials rather than divisions (d). Thanks to this change, P<sup>i</sup> curves of different electrons can be added or calculation centred on concrete r<sup>i</sup> can be made.

## **KEYWORDS**

NIN coupling, Electron Probability, Origin Electronic System (OES), Born Electronic System (BES), Victoria Equation.

## **INTRODUCTION**

This is  $7<sup>th</sup>$  article of 24 dedicated to atomic model based on Victoria equation (Articles index is at end). A extern electronic extreme ( $EE_A$ ) is indicated with a suffix  $(r_A, H_A \text{ or } t_A)$  $c_A$ ), B intern with b suffix ( $r_B$ ,  $h_B$  or  $c_B$ ) and i suffix is used to both electronic extremes (EEi). All abbreviations are compiled, in conjunction with those included in [6], at article end.

Electron with two EE has been introduced by Victoria Equation [1] and has been developed its geometry and probability [2-6] until achieving geometric and probabilistic coupling according to P34 NIN III [6]. This coupling between electron lobes (or Electronic Systems) by NIN rules allows extern electrons to be positioned by ns origin and provides approximate maximum electron density in n as  $P_i$  maximum contributed by the outermost Electronic System in n.

If in  $[6]$  maximum  $P_i$  is approximated by visual method from Pi vs. ri curve or from data with which figures have been made, curves overlap by P34 NIN III and maximum electron density are now studied in more detail using delimited  $r_i$  differentials. Initially, this study is centred on Oxygen lobes in n=2 to be later amplified to rest of atoms and lobes.

z,  $C_{PEP}$  and  $C_{POTI-AL}$  (P32  $C_{POTI}$  angular limit [5]) are calculated according [6] and summarized in P34 NIN III.

#### **Born z by z coupling**

Born Electronic System z (BES z or  $z_B$ ) is provided by "P41 Electronic Charge (z) Coupling" [6] (1). Where BES is non-origin lobe and origin lobe is only ns electron external lobe. OES z or z<sub>O</sub> is Origin Electronic System z.

$$
(1)\ z_\text{B}=z_\text{O}(\frac{(E_\text{o})_\text{B}}{(E_\text{o})_\text{O}}
$$

(1) relates to ns origin electronic system (OES) because is the first in n quantum number and its z is known (P14 Effective nuclear charge in ns electrons [1]) and on which the rest are grouped. Anyway, all formulas that indicate O (Origin) and B (Born) can be transformed by considering born lobes  $(X \text{ and } Y)$  that are located on the same n  $(2)$ 

$$
(2) \ z(Y) = z(X) \, \frac{(E_\circ)_Y}{(E_\circ)_X}
$$

P14 Effective nuclear charge in ns electrons, which subtracts one charge for each extern electronic system as loses energy, is only a good approximation when z and energy relations are in concordance (3). Where  $z_B^*$  is  $z_B$ , but applying P14 to system not OES.

$$
(3) \frac{\text{zo}}{\text{Z}_\text{B}^*} \approx \frac{\text{I}\text{E}_\text{O}}{\text{I}\text{E}_\text{B}}
$$

P14 is correct with ns external lobe and a good estimate when is applied on  $\text{ns}^2$  external lobe. Applying P14, ns<sup>2</sup> has one unit less charge that ns since  $\text{ns}^2$  is next in energy after ns (**Table 1**).



Considering (3) and accepting P14 for  $ns^2$ , Ionization Energy (IE) (experimental data in [7]) and Charge (z) ratios between ns and  $ns<sup>2</sup>$  electronic system are represented in **Figures 1 and 2** for n=2 and n=3 respectively. In both n quantum numbers, there is good overlap between two relationships. This fact implies that applying P14 to estimate ns<sup>2</sup> external lobe charge is a good approximation and can be corroborated with **Table 2** where z has been obtained by P41 (1). However, if this is done on 2p lobe where an additional unit of charge must be subtracted according to P14, **Figure 3** is obtained with a bad overlap between two ratios which is checked in Table 2. Charge correct values are in Table 2 for all electronic systems (lobes) located on n=2 of atoms with 2s electron having  $z = [1-8]$ .







## **CPOTI-AL Coupling**

Probabilistic Orbital Tide Coefficient (C<sub>POTI</sub>) is introduced in P30 Third Feliz Solution [5]. C<sub>POTI</sub> can reach up to C<sub>POTI</sub> Maximum Geometric Angular Limit or C<sub>POTI</sub> Angular Limit (C<sub>POTI-AL</sub>) when nucleus-orbit-angle ( $\alpha_{NOA}$ ) is 180 degrees and can not be overcome (P32) except by  $C_{POTI-AL-d\rightarrow\infty}$  hypothesis [5]).  $C_{POTI-AL}$  by division with  $C_{POTI}$ minimum [5] is employed (4):

$$
(4) \ C_{\text{POTIMinimum}} = \frac{\sqrt{2m_{\text{e}}f\mathbf{z}}}{\hbar} \, r_{\text{i}}^{\text{1/2}} C_{\text{MON}}
$$

 $C_{POTI}$  minimum is located in B intern electronic extreme by division (d) inclusion that provide  $C_{MON}$  and  $r_i$  values. 2s Nitrogen in its outermost lobe (n=2) has been taken by way of example. Division differences of 1 and 0.05 are chosen to observer consequent difference in minimum  $C_{POTI}$  obtained in (4) ( $C_{POTI-AL}$ ). P14 can be used because 2s Nitrogen is origin lobe and therefore  $z=7-2=5$  (Table 2). MON=10 according to P37.C. [6]. Search for C<sub>POTI</sub> minimum can be performed considering this information and experimental IE [7]. Data are summarized in **Table 3**.



Difference between d with  $H\rightarrow 0$  is appreciable (20 and 19,55), although implies an effect on limited C<sub>POTI-AL</sub> (difference $\approx 6*10^{-5}$ ). This difference in C<sub>POTI-AL</sub> estimation is even lower if d is higher since d increase implies smaller magnitude differences between divisions.

CPOTI-AL for lobes in  $n=2$  from Li to Ne are in Table 4. 2s in  $n=2$  (OES) is obtained by method of CPOTI-AL by division with CPOTI minimum and rest of Electronic Systems in  $n=2$  (BES) is approximated with (5). (5) is given by P43 C<sub>POTI</sub> coupling [6].

$$
(5) \ C_{\text{POTI - B}} = C_{\text{POTI - O}} \ \sqrt{\frac{(E_{\circ})_B}{(E_{\circ})_O}}
$$





Divisions, with accuracy  $= 0.01$ , that hold OES C<sub>POTI-AL</sub> are in **Table 5**. MON (P37 [6]) are also included in this Table 6. If MON is equal, divisions for CPOTI-AL are similar and with a slight increasing trend with Atomic number. This MON influence in division that

has C<sub>POTI-AL</sub> evidences MON importance in morphology of geometric and probabilistic curves and therefore in CPOTI-AL.

## **MON Coupling**

OES MON is supplied by "P37 OES MON" and BES MON is provided by "P39 MON Coupling" [6] (6). MON for lobes in n=2 from Li to Ne are in **Table 6**.

$$
(6) \, MON_B = MON_0 \frac{(E_o)_o}{(E_o)_B}
$$



## **CPEP Coupling**

BES CPEP is given by (7) according to "P42 CPEP as adapted Probability between a electrons pair". 2s OES CPEP is taken equal to 1 because BES are born lobes whose Probability (Pi) are compared to OES. C<sub>PEP</sub> is in **Table 7** for lobes in n=2 from Li to Ne.

(7) 
$$
C_{\text{PEP(Bto O)}} = \sqrt{\frac{(E_{\text{o}})_{\text{o}}}{(E_{\text{o}})_{\text{B}}}}
$$
 For  $P_{B \text{ to O}}$  (P<sub>BORN TO ORIGIN</sub>)





#### **H<sup>i</sup> vs P<sup>i</sup> representation with CPEP=1**

 $H_i$  is circular orbital height.  $P_i$  and EE orbital circumference  $(c_i)$  are closely related through Compaction Factor (CF) [3-6]. Thus,  $H_i$  vs  $P_i$  is an approximation to  $H_i$  vs  $c_i$ and, consequently, provides an orbital geometry idea in two dimensions (height and width). Turn with radius=c<sub>i</sub> allows to reach 3 dimensions. H<sub>i</sub> vs  $P_i$  and not  $P_i$  vs H<sub>i</sub> is for this reason of indirect geometric representation.

In **Figure 4 and 5** are A and B electronic extremes that correspond to electron in Oxygen that is in each one of six electronic systems that Oxygen have in n=2. In all lobes C<sub>PEP</sub>=1, i.e. no C<sub>PEP</sub> coupling, to observe initial positions before being referred to OES. Consequently, P34 NIN III is only with Geometric NIN Coupling (GNC) [6]. Figure 5 differs from 4 in that Y axis is enlarged from 0.3 to 1 A to achieve a broader view of the curve shape.





From both figures can be highlighted:

1) Electronic systems with higher IE present curves with  $P_i$  lower. Even considering that BES z are not integer (P41 [6]), order in  $P_i$  is deductible for their energies. Thus, curves located from lowest to highest probability are:

$$
2s<2s^2<2p<2p^2<2p^3<2p^4\\
$$

2) Curves shape is very similar although curves width differs. Role for Probabilistic NIN Coupling (PNC) is assumed by  $C_{PEP}$  (P34 NIN III [6])

3) In addition to similar curves shape, there are two geometric points that allow to imagine PNC:

3.1) Curves are linked at low  $d_B$  (where B subscript refers to B intern electronic extreme) See in Figure 4.

3.2) Division infinite points in  $H_i$  vs  $P_i$  representation are aligned with identical H<sup>i</sup> fulfilling division infinite coupling between lobes (electronic systems) located in same n. In **Figure 6**, this  $H_i$  can be located above  $7,55 \cdot 10^{-12}$  m and can be specified with numerical treatment around  $7,561 \cdot 10^{-12}$  m.



## **P<sup>i</sup> vs. r<sup>i</sup> representation with CPEP=1**

Unlike the previous point,  $P_i$  is in Y axis since is  $r_i$  function. Also, is classic location in bibliography. Lobes are adjusted with GNC (**Figure 7** with C<sub>PEP</sub>=1) as has been done in previous point with  $H_i$  vs.  $P_i$ . PNC view is represented later.  $P_i$  maximum varies slightly from 2s OES to the outermost  $2p^4$  BES which is located at  $\approx$  46 pm and agrees with 46 pm [8] and 44 pm [9]. Fluorine [6] and Oxygen have same 2s OES MON=10 (P37 [6]) and their P<sup>i</sup> maxima are correlated with those contributed by references. Outermost BES  $P_i$  is taken as  $P_i$  maximum for n quantum number where this outermost BES is located in a first approximation because:

1)  $2p<sup>4</sup>$  Outermost BES has a much higher probability than internal lobes as 2s OES. Specifically, in Oxygen case is on order of 3 times higher provided is assumed that global probability is referred to  $C_{PEP}=1$ . This model with GNC is compared in the following article with probability calculation when PNC has been produced.

2) Usually, there are more external electrons than internal electrons. In this case, there are 4 in 2p and 2 in 2s.

3) Curves and maxima are similar and therefore, differences between models are reduced.



Calculation method with  $r_i$  defined - Application to Probability

(8) subsequent use is indicated in [1]. (8) permits to know division associated with  $r_A$ and therefore r<sub>A</sub> specific region can be studied.

$$
(8) d = \frac{E_o \lambda + \frac{F \lambda}{2r_A}}{F + E_{oI_A}}
$$

1) Lobe Individual  $P_i$  (C<sub>PEP</sub>=1)

For  $n=2$ ,  $2s^2$  and  $2p^4$  Probability is in **Figure 8**. Figure 8 is bounded between 35 and 52 pm with  $r_i=0,5$  pm variations. Maxima of both lobes are very close. This fact can be corroborated by **Figure 9** and **10** and corresponding **Table 8 (Annex)** where maxima have been highlighted.  $P_i$  vs.  $r_i$  representations for  $2s^2$  and  $2p^4$  are in Figure 9 and 10 respectively.

 $2)$  Lobes P<sub>i</sub> Sum (C<sub>PEP</sub>=1)

Following steps are in this model:

2.1) Lobes that exist in a concrete n.

2.2)  $P_i$  vs.  $r_i$  curves for each lobe. All curves with  $C_{PEP}=1$ 

2.3) Multiply  $P_i$  by electrons number that have that lobe; i.e. consider its electronic configuration (Oxygen  $n=2$  shell has 2 electrons with lobe  $2s<sup>2</sup>$  and 4 electrons with lobe  $2p^4$ ).

2.4) Lobes  $P_i$  summation. In Oxygen n=2 shell case, lobes  $P_i$  summation is represented in **Figure 11**. Resulting curve is similar to individual ones and has no discontinuities. P<sub>i</sub> maximum is located at  $\approx$  46 pm and is also in agreement with 46 pm [8] and 44 pm [9].



 $P_i$  vs.  $r_i$  curves can be constructed with lower  $r_i$  differentials to have a greater precision. Lobes  $P_i$  sum with C<sub>PEP</sub> coupling (PNC) can be studied although resulting curve and  $P_i$ Maximum have little variation with what is seen at this point. Variations are somewhat greater when n quantum number increases, implying that MON decreases (P37 [6]) and P<sup>i</sup> vs. r<sup>i</sup> curves are diverted to higher ri. These points are expanded in following article.

# **P<sup>i</sup> representations with CPEP Coupling (Probabilistic Nin Coupling or PNC)**

Above curves are transformed into PNC by CPEP coupling. Data for CPEP Coupling in oxygen  $n=2$  shell are in **Table 7**.  $P_i$  vs.  $r_i$  representation with PNC for its six electronic systems is in **Figure 12**. All electronic systems are overlapped in infinite division and in wide range of B intern electronic extreme. With respect to A extern electronic extreme, curves overlap is performed up to near  $P_i$  maxima zone, from where distancing between P<sup>i</sup> curves begins to become more noticeable as lobes are more energetically distanced (**Figure 13**).

H<sub>i</sub> vs. P<sub>i</sub> representation is in **Figure 14**. C<sub>POTI-AL</sub> Coupling has been obtained from Table 4. Electronic extremes births junction is  $H_i \approx 7.5$  pm as discussed previously. If instead of working with  $C_{POTI-AL}$  and its  $\alpha_{NOA}=180$  degrees, lower OES  $C_{POTI-GAI}$  is selected, PNC is maintained.





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#### **Abbreviations List**

Suffix indicates electronic extreme considered and i suffix is used to both electronic extremes (EEi). Following Table indicates abbreviations used in this theory and its use in article in question is marked with X. 7 is present article. Jump from "Article 09" to "Article 20" is consequence of second part inclusion.







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#### **Annex**



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